Study of interactions between single walled carbon nanotubes and a flagellin-specific library of tripeptides

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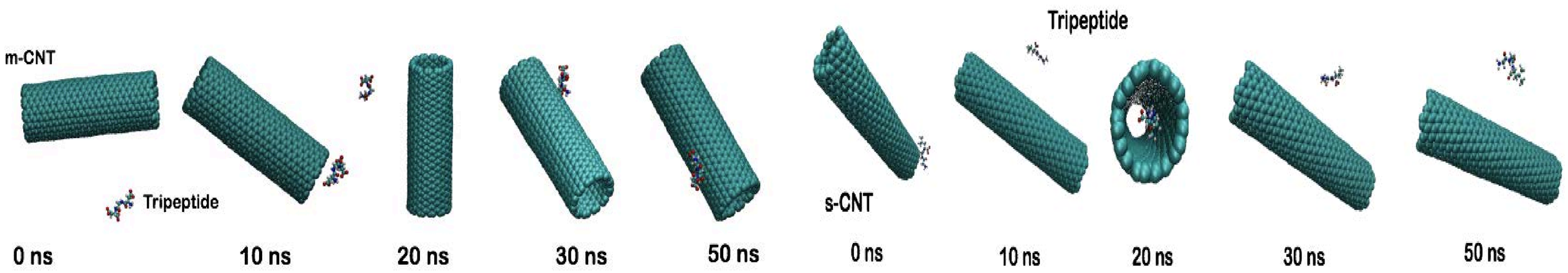
VMD



Abstract

Dispersion of single walled carbon nanotube in water is hard to achieve due to the strong cohesive forces existing between them. A good dispersion of nanotubes is essential for their separation into their chirality based separation. Many surfactants like SDS have been used to create a dispersion of nanotubes and for their separation into different chiralities (zig-zag, armchair and chiral). The dual action of these surfactants is assumed to be due to their amphiphilic nature of a hydrophobic core surrounded by a hydrophilic head. The interaction of carbon nanotubes with biological molecules has been less studied hence finding peptides which can disperse the bundle or ropes of nanotube while displaying selective affinity for different kinds of nanotube can expand the small list of surfactants existing today. In this study, we create a tripepetide library from the D3 domain of flagellin (used in previous study by Macwan *et al*.) All the 9 tri-peptides in the library showed the presence of a middle glycine residue. Their interactions with single walled carbon nanotubes was studied using Visual Molecular Dynamics (VMD). **RMSD** provided quantitative and qualitative data to determine the extent and selectivity of the interactions, hence allowing us to screen the tri-peptide library to determine the tri-peptides with the best selective affinitv for the nanotubes.

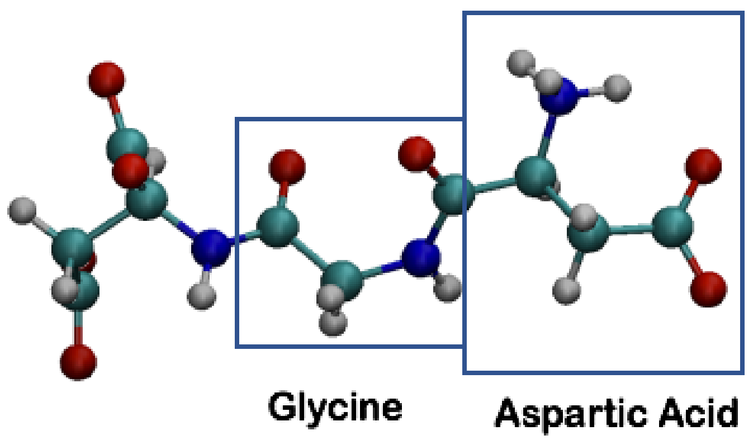


Figure 1: *Nine such tri-peptides with glycine as the middle residue is forms the tri-peptide library.*

Tripeptide Library Combinations:

1. Threonine-Glycine-Tyrosine
2. Aspartic Acid-Glycine-Tyrosine
3. Asparagine-Glycine-Glutamic Acid
4. Aspartic Acid-Glycine-Aspartic Acid
5. Threonine-Glycine-Glycine

Tripeptide Library Combinations:

6. Glycine-Glycine-Leucine
7. Threonine-Glycine-Lysine
8. Glycine-Glycine-Alanine
9. Glycine-Glycine-Leucine

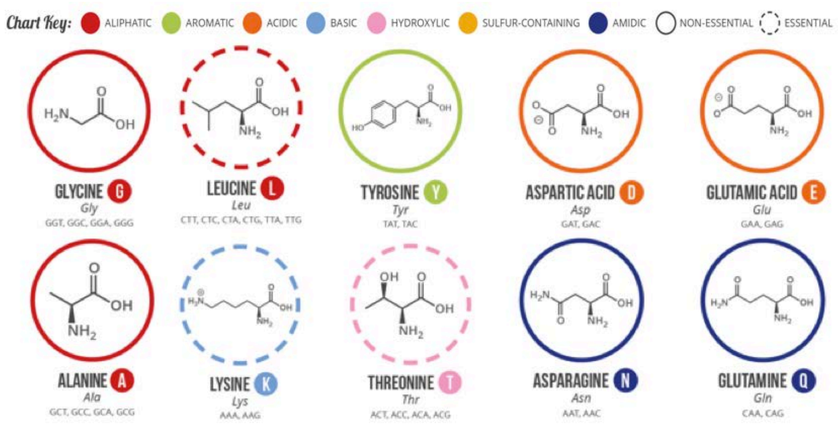


Figure 2: *Physical properties of each amino acid residue present in the nine combinations. Their physical properties are the extent of hydrophilicity or lipophilicity hence modulating their surfactant behavior.*

Methodology

Molecular Dynamics based simulations were carried out using VMD and NAMD. R-type falgellin pdb (1UCU) file was obtained from the Protein Data Bank. Tri-peptides were extracted from the D3 domain of R-type flagellin pdb file. Simulations were carried out between armchair (m-CNT) and zig-zag (s-CNT) form of single walled CNT and the tripeptide library for a period of 50 ns. All simulations used the CHARRM force field, TIP3 water model and a 0.05 mol/l neutralizing NaCl concentration. Temperature was maintained at 300 K at a pressure of 1 atm.

Results

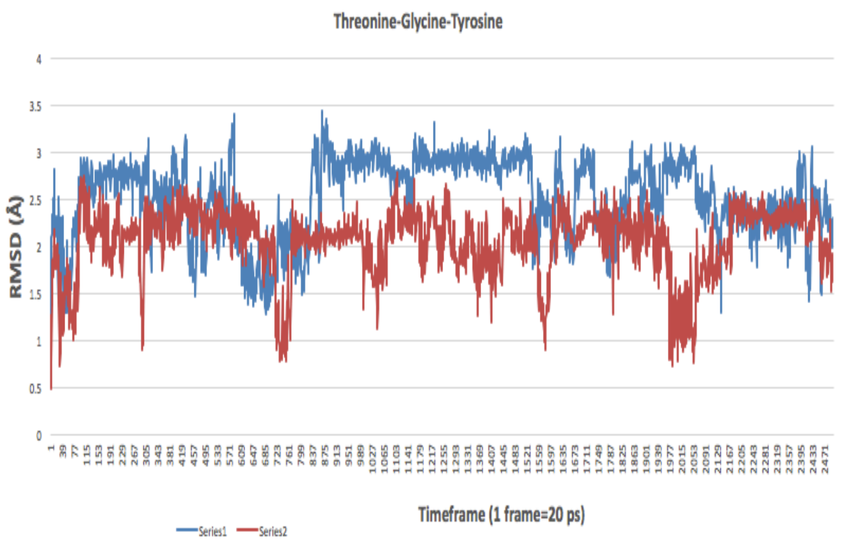


Figure 3: *RMSD between Threonine-Glycine-Tyrosine tripeptide and SWCNT of both armchair (blue) and zig-zag/chiral (red) form.*

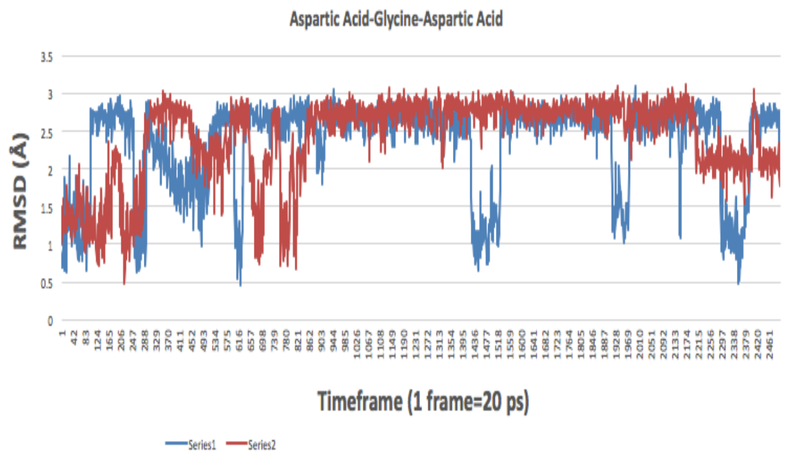


Figure 4: *RMSD between Aspartic Acid-Glycine-Aspartic Acid tripeptide and SWCNT of both armchair (blue) and zig-zag/chiral (red) form. The RMSD stabilizes by timeframe 2200.*

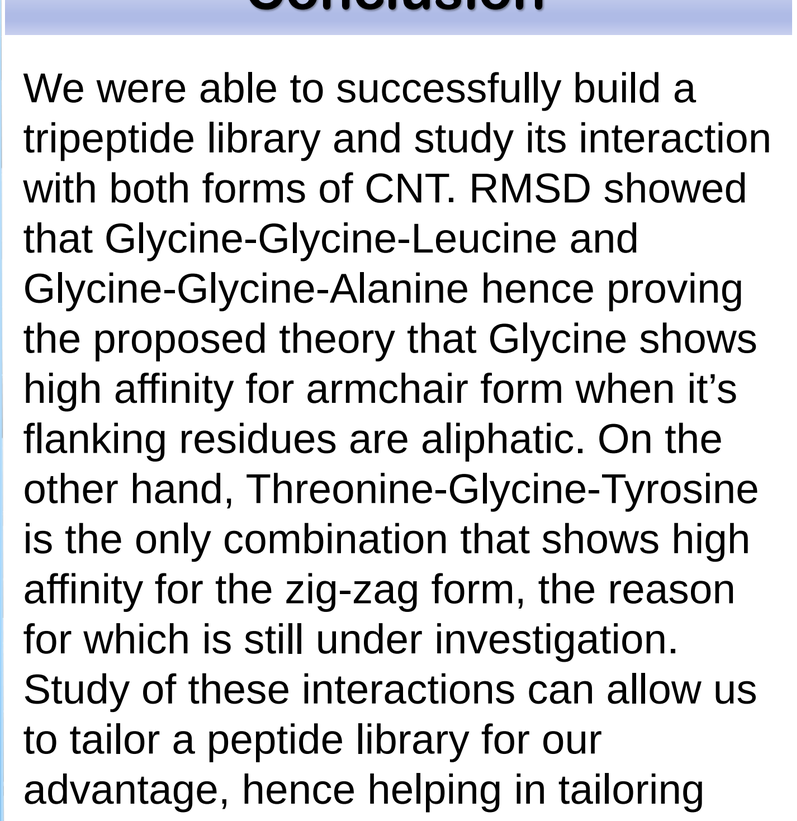


Figure 5: *Comparison between the different combinations of tripeptides in the library for both armchair (blue) and zig-zag/chiral (red) form of CNT.*

Conclusion

We were able to successfully build a tripeptide library and study its interaction with both forms of CNT. RMSD showed that Glycine-Glycine-Leucine and Glycine-Glycine-Alanine hence proving the proposed theory that Glycine shows high affinity for armchair form when it's flanking residues are aliphatic. On the other hand, Threonine-Glycine-Tyrosine is the only combination that shows high affinity for the zig-zag form, the reason for which is still under investigation. Study of these interactions can allow us to tailor a peptide library for our advantage, hence helping in tailoring systems which are driven by forces. The experiments of this study is underway.

References

1. Macwan, I. *et al.* Residue Specific and Chirality Dependent Interactions between Carbon Nanotubes and Flagellin. *IEEE/ACM Trans. Comput. Biol. Bioinforma.* **5963,** 1–1 (2015).
2. Wang, S. *et al.* Peptides with selective affinity for carbon nanotubes. *Nat. Mater.* **2,** 196–200 (2003).